

# Four flavour simulations with maximally twisted mass QCD

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for the **European Twisted Mass Collaboration**



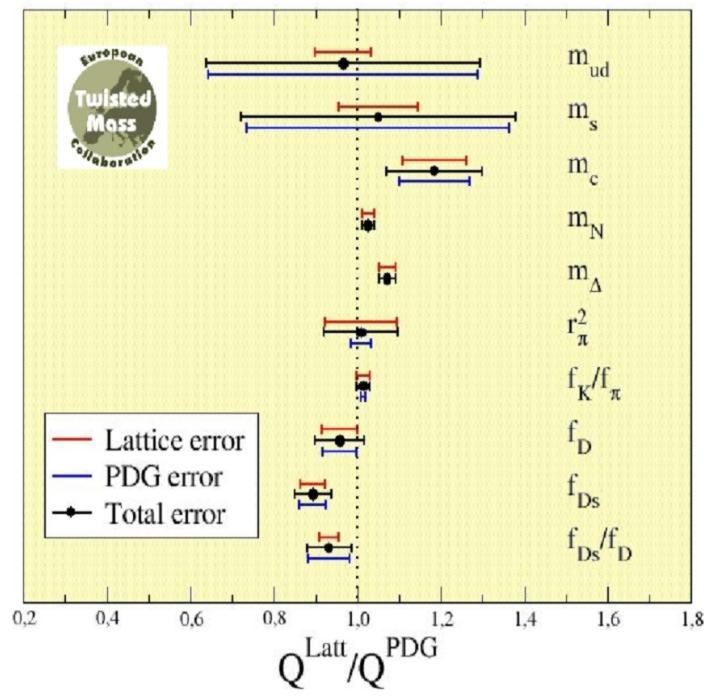
- Twisted mass fermions
- Selected results for  $N_f = 2 + 1 + 1$  flavours
- A glimpse at our next plans



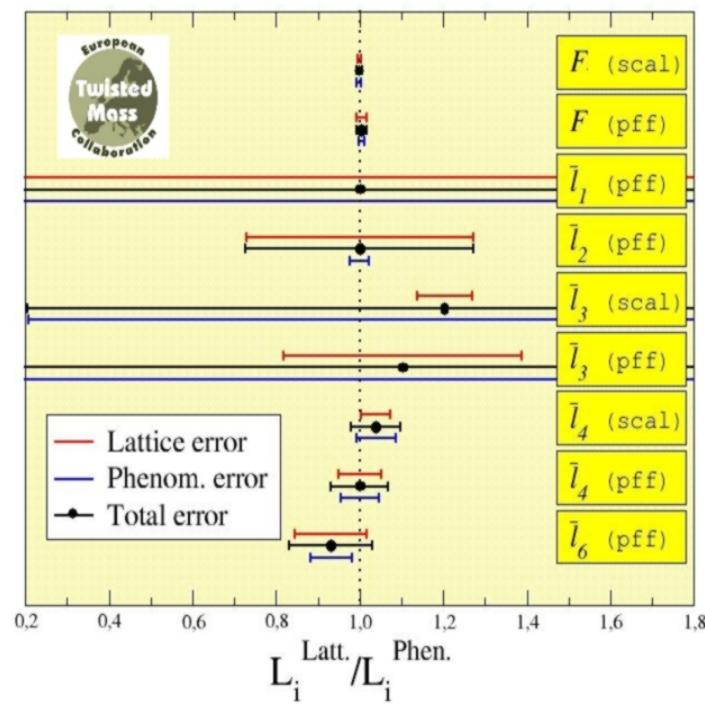
- **Cyprus (Nicosia)**
- **France (Orsay, Grenoble)**
- **Italy (Rome I,II,III, Trento)**
- **Netherlands (Groningen)**
- **Poland (Poznan)**
- **Spain (Huelva, Madrid, Valencia)**
- **Switzerland (Bern)**
- **United Kingdom (Glasgow, Liverpool)**
- **Germany (Berlin/Zeuthen, Bonn, Frankfurt, Hamburg)**

Collaboration performed very successful  $N_f = 2$  research programme

## Simulation results versus PDG



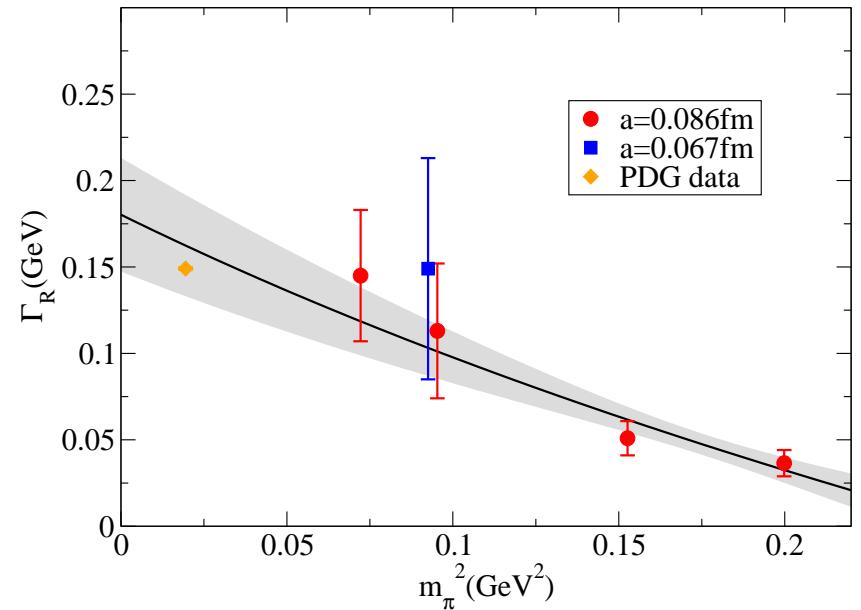
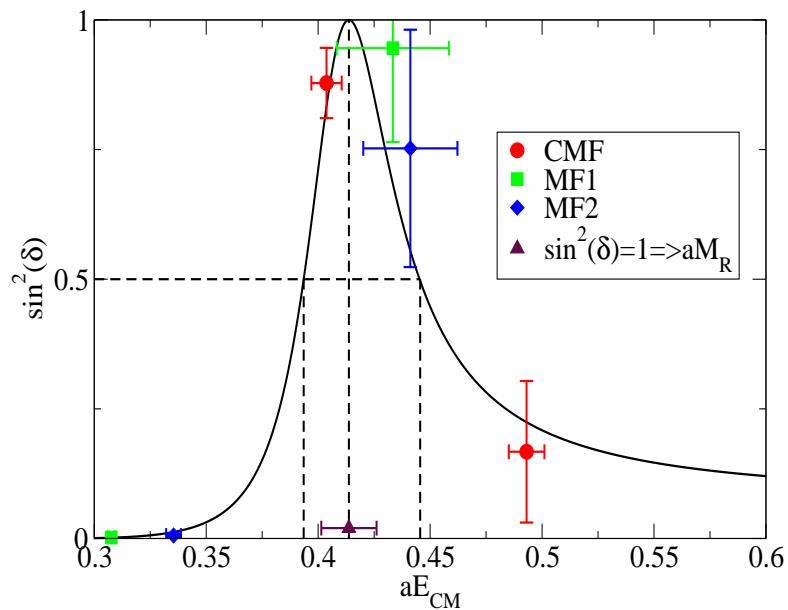
## Low energy constants



# The $\rho$ -meson resonance: dynamical quarks at work

(X. Feng, D. Renner, K.J.)

- usage of three Lorentz frames



$$m_{\pi^+} = 330 \text{ MeV}, a = 0.079 \text{ fm}, L/a = 32$$

$$\text{fitting } z = (M_\rho + i\frac{1}{2}\Gamma_\rho)^2$$

$$m_\rho = 1033(31) \text{ MeV}, \Gamma_\rho = 123(43) \text{ MeV}$$

## Natural<sup>2</sup> next step: move to four flavours

- twisted mass: works with quark doublets
  - maximal twist: automatic  $O(a)$ -improvement
  - infrared cut-off due to twisted quark mass
  - simplification in renormalization ( $f_\pi$ ,  $\langle N | \bar{q}q | N \rangle$ )
- ★ ★ ★ need to control isospin splitting effects
- strange and charm quarks needed for physical quantities
  - mesons:  $m_{\text{strange}}$ ,  $m_{\text{charm}}$ ,  $f_D$ ,  $f_{D_s}$ ,  $\eta'$ ,  $\eta_c$
  - baryons: spectrum,  $\langle N | \bar{q}q | N \rangle$
  - $g_\mu - 2 \leftarrow$  can unambiguously compare to experimental value
  - running of  $\alpha_{\text{strong}}(\mu)$  with four flavours

## Wilson (Frezzotti, Rossi) twisted mass QCD (Frezzotti, Grassi, Sint, Weisz)

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Fermion action of twisted mass fermions

$$S_l = \sum_x \bar{\chi}_x^l \left[ m_q + \frac{1}{2} \gamma_\mu [\nabla_\mu + \nabla_\mu^*] - a \cancel{r} \frac{1}{2} \nabla_\mu^* \nabla_\mu + i \cancel{\mu}_{\text{tm}} \tau_3 \gamma_5 \right] \chi_x^l$$

$$S_h = \sum_x \bar{\chi}_x^h \left[ m_q + \frac{1}{2} \gamma_\mu [\nabla_\mu + \nabla_\mu^*] - a \cancel{r} \frac{1}{2} \nabla_\mu^* \nabla_\mu i \gamma_5 \tau_1 \cancel{\mu}_\sigma + \tau_3 \cancel{\mu}_\delta \right] \chi_x^h$$

- quark mass parameter  $m_q$ , twisted mass parameter  $\mu_{\text{tm}}$
- strange and charm quark masses

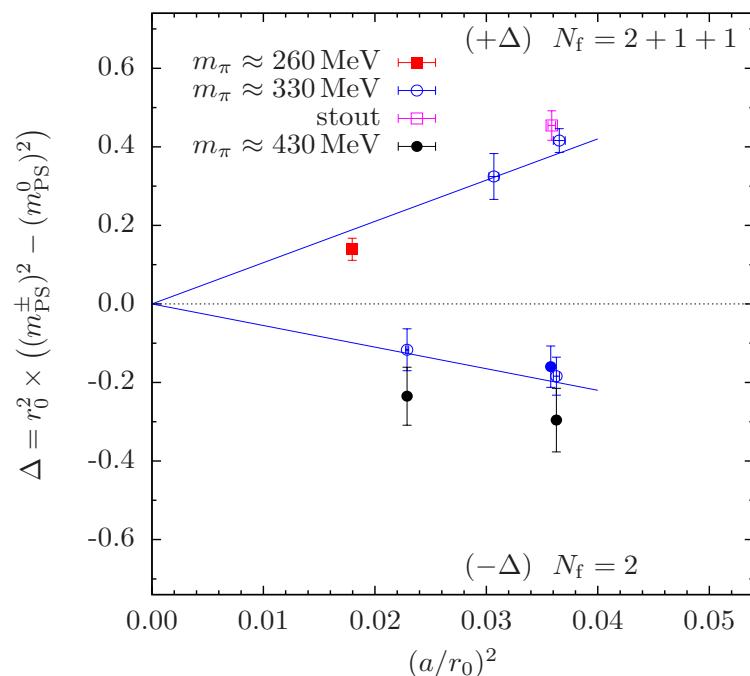
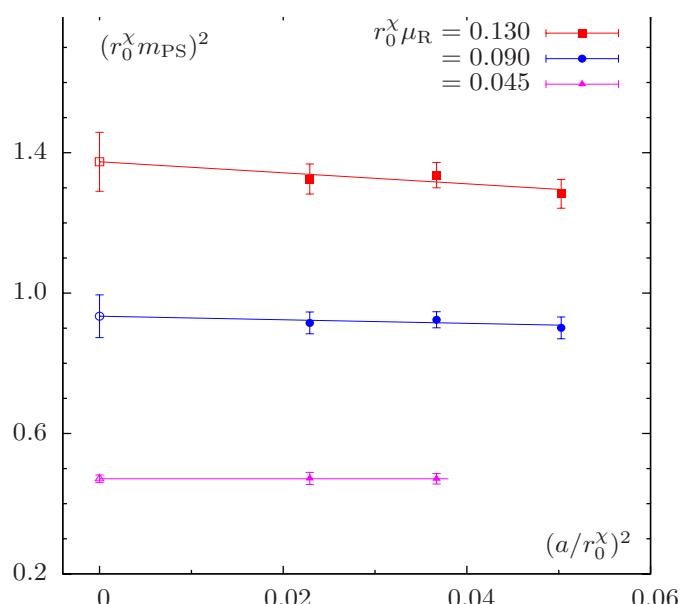
$$m_s = Z_P^{-1} \mu_\sigma - Z_S^{-1} \mu_\delta$$

$$m_c = Z_P^{-1} \mu_\sigma + Z_S^{-1} \mu_\delta$$

- note,  $m_q$  the same in  $S_l$  and  $S_h$

## A word on flavour breaking

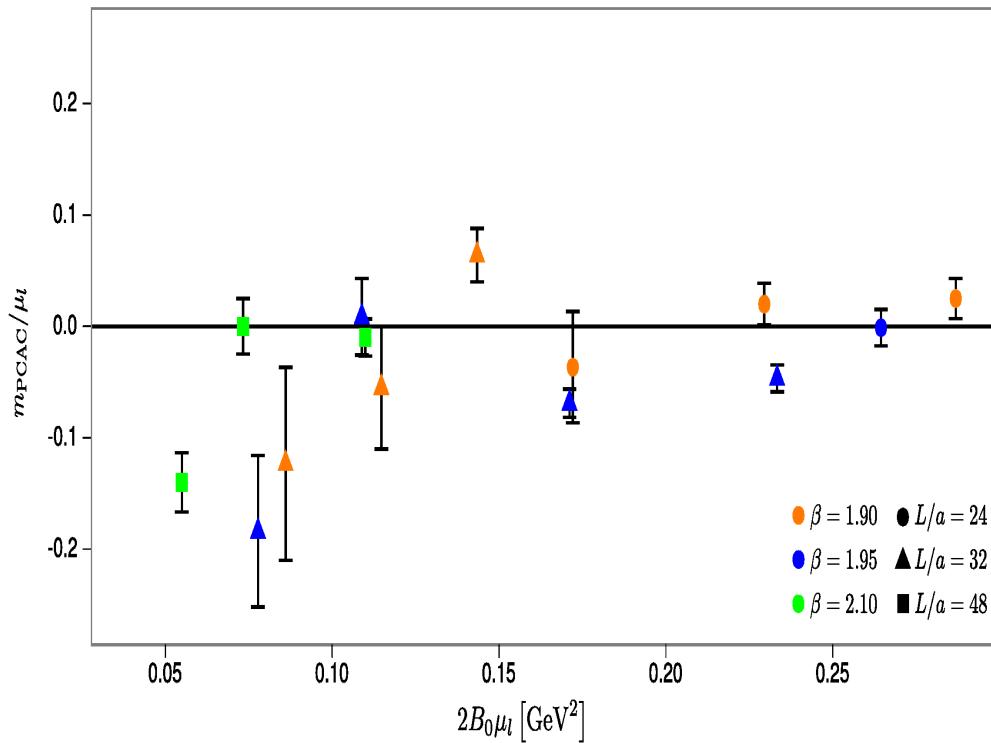
- isospin (flavour symmetry) violation at any  $a \neq 0$ :  $m_\pi^\pm - m_\pi^0 \neq 0$
- observe large  $\mathcal{O}(a^2)$  effect in neutral pion mass
- effect visible both for  $N_f = 2$  and  $N_f = 2 + 1 + 1$
- theoretical understanding (Dimopoulos et.al., Phys. Rev. D81, 034509 (2010))
- $\chi$ PT analysis of meson sector including pion mass splitting  $a^2$  effect  
(O. Bär, Phys.Rev. D82 (2010) 094505)



## Tuning to maximal twist

Maximal twist: tune  $m_q$  such that

$$m_{\text{PCAC}} = \frac{\sum_x \langle \partial_0 A_0^a(x) P^a(0) \rangle}{2 \sum_x \langle P^a(x) P^a(0) \rangle} = 0$$



- tuning of  $m_q$  at each  $\mu_{\text{tm}}$  used
- demand  $m_{\text{PCAC}} \lesssim 0.1 \mu_{\text{tm}}$
- demand  $\Delta(m_{\text{PCAC}}) \lesssim 0.1 \mu_{\text{tm}}$

## Autocorrelations from gradient flow

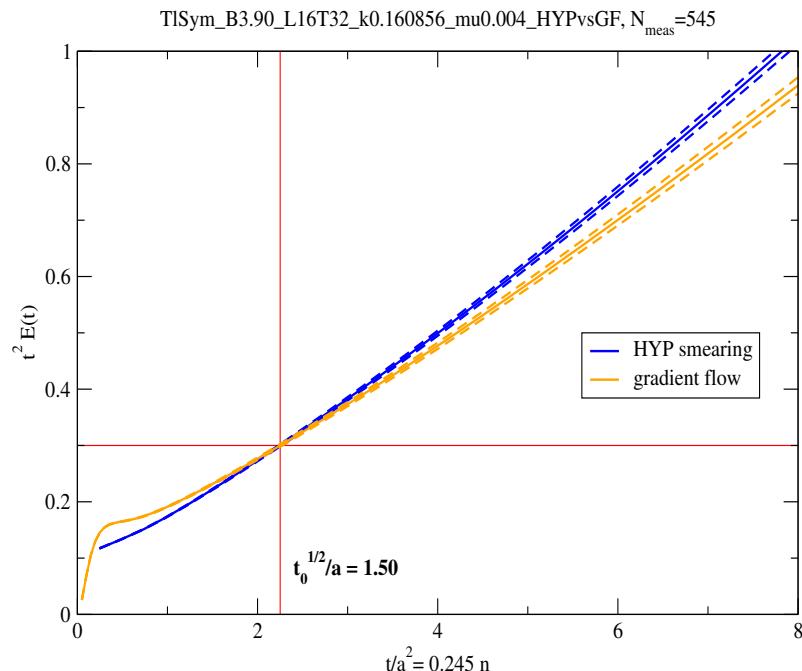
(Deuzemann, Wenger) see also talk by Z. Fodor

- flow of the gauge field  $U(x, \mu)$  according to the flow equation

$$\frac{\partial}{\partial t} V_t(x, \mu) = -g_0^2 \{ \partial_{x,\mu} S_{\text{latt}} W(V_t) \} V_t(x, \mu)$$

$$V_{t=0}(x, \mu) = U(x, \mu)$$

- lattice: discrete integration scheme with *finite step size*  $\epsilon$  for integration



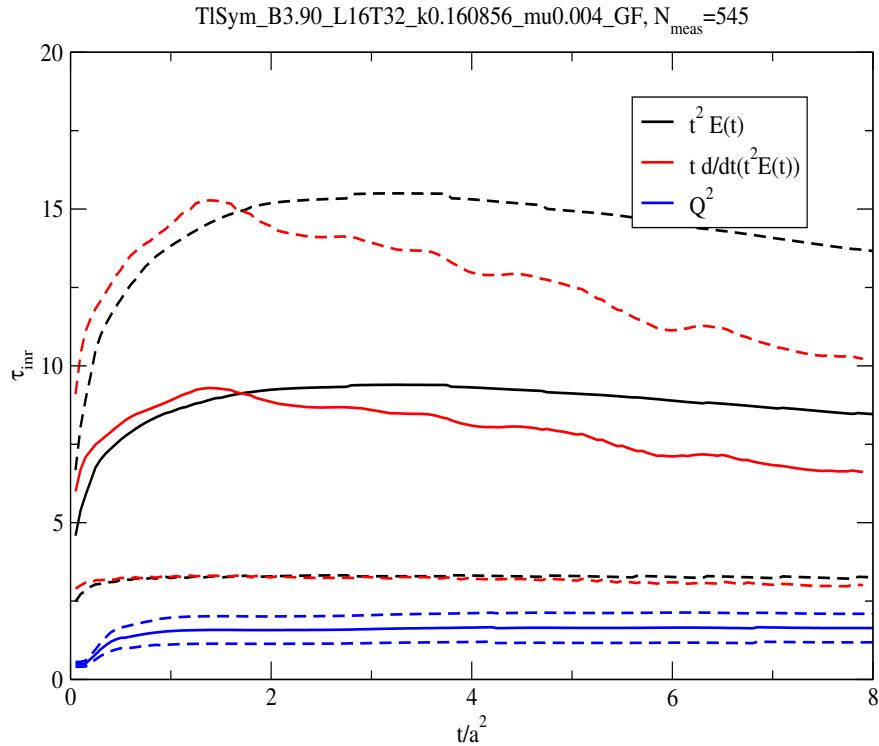
$$a \approx 0.08 \text{ fm} \quad m_\pi \approx 300 \text{ MeV}$$

energy density:

$$E(t) = 2 \sum_{\text{plaq}} \text{Retr}[1 - V_t(\text{plaq})]$$

## Topology and autocorrelations

- topological charge well defined on smooth configurations  $V_t$
- use standard field theoretic definition  $F_{\mu\nu}\tilde{F}_{\mu\nu}(V_t)$

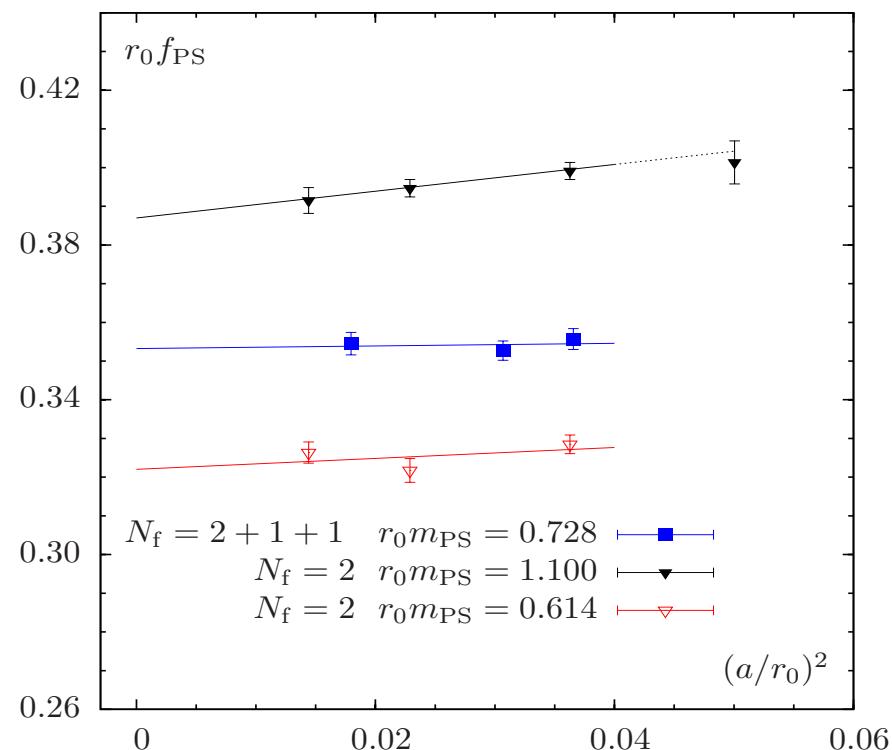


gradient flow gives largest autocorrelation

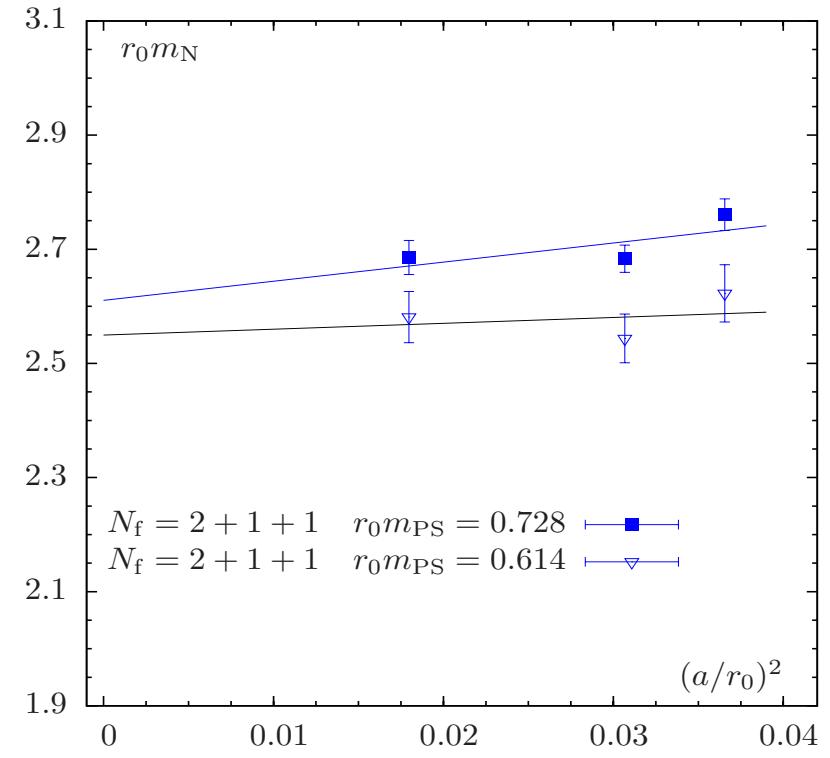
autocorrelation from topological susceptibility significantly smaller

★ ★ ★ warning

## $N_f = 2 + 1 + 1$ light quark sector: scaling



pseudoscalar decay constant  $f_{\text{PS}}$



nucleon mass

$$N_f = 2 + 1 + 1 \text{ light quark sector: } \chi\text{PT fit}$$

- basic formulae:  $N_f = 2$  continuum  $\chi\text{PT}$  at NLO

$$m_{\text{PS}}^2 = \chi_\mu [1 + \xi \log(\chi_\mu/\Lambda_3^2)] K_m^2(L)$$

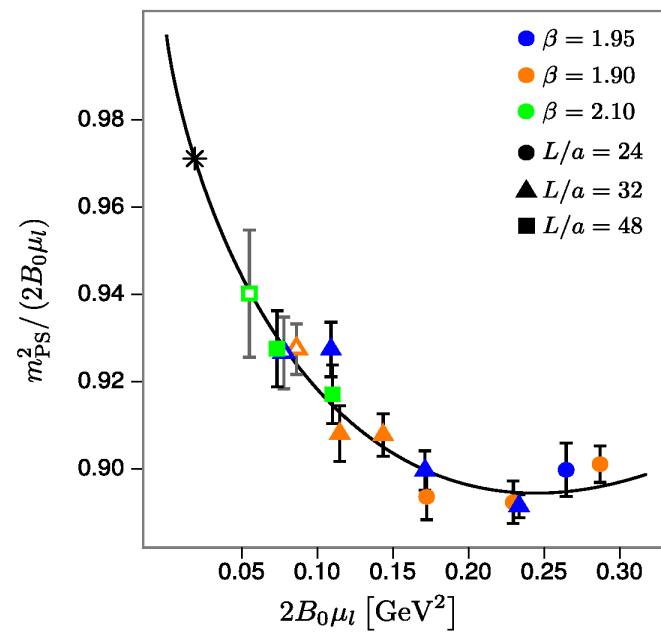
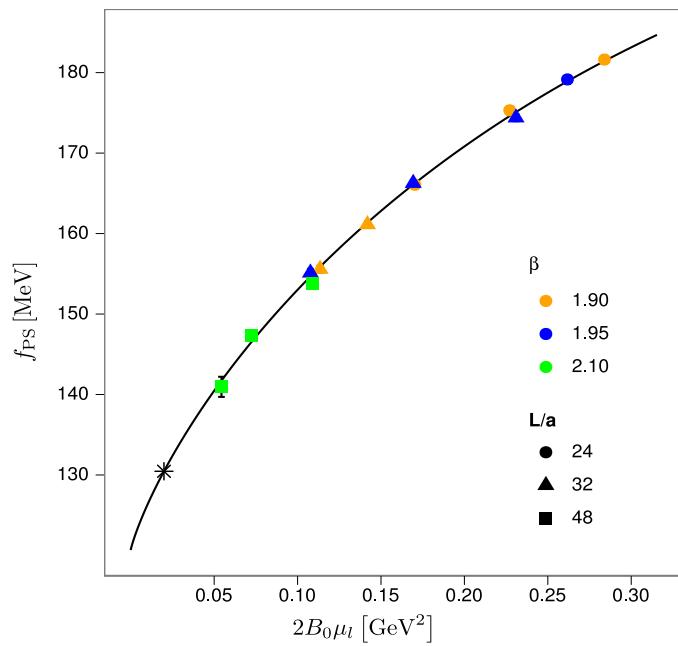
$$f_{\text{PS}} = f_0 [1 - 2\xi \log(\chi_\mu/\Lambda_4^2)] K_f(L)$$

$$\chi_\mu = 2\hat{B}_0 Z_\mu \mu_q , \quad \xi = \chi_\mu / (2\pi f_0)^2$$

- finite size corrections  $K_m(L), K_f(L)$   
(Gasser, Leutwyler, 1987, 1988; Colangelo, Dürr, Haefeli, 2005)  
in preparation: analysis a la Colangelo, Wenger, Wu; Bär; Ueda, Aoki
- fit simultaneously to our data at all  $\beta$ -values
- fit includes renormalisation constant  $Z_\mu = 1/Z_P$

## $N_f = 2 + 1 + 1$ light quark sector: $\chi$ PT fit

- estimate systematic effects : lattice artifacts, FSE



## Comparison of low energy constants

	$N_f = 2$	$N_f = 2 + 1 + 1$
$\bar{\ell}_3$	3.70(27)	3.50(31)
$\bar{\ell}_4$	4.67(10)	4.66(33)
$f_\pi/f_0$	1.076(3)	1.076(9)
$B_0$ [MeV]	2437(120)	2638(200)
$\langle r^2 \rangle_s^{\text{NLO}}$ [fm $^2$ ]	0.710(28)	0.715(77)

## $N_f = 2 + 1 + 1$ adding strange quark: fit formulae

- $SU(2)$   $\chi$ PT Fit Formulae for  $f_K$  and  $f_\pi$ :

$$f_{\text{PS}}(\mu_\ell, \mu_\ell, \mu_\ell) = f_0 \cdot (1 - 2 \xi_{\ell\ell} \ln \xi_{\ell\ell} + b \xi_{\ell\ell})$$

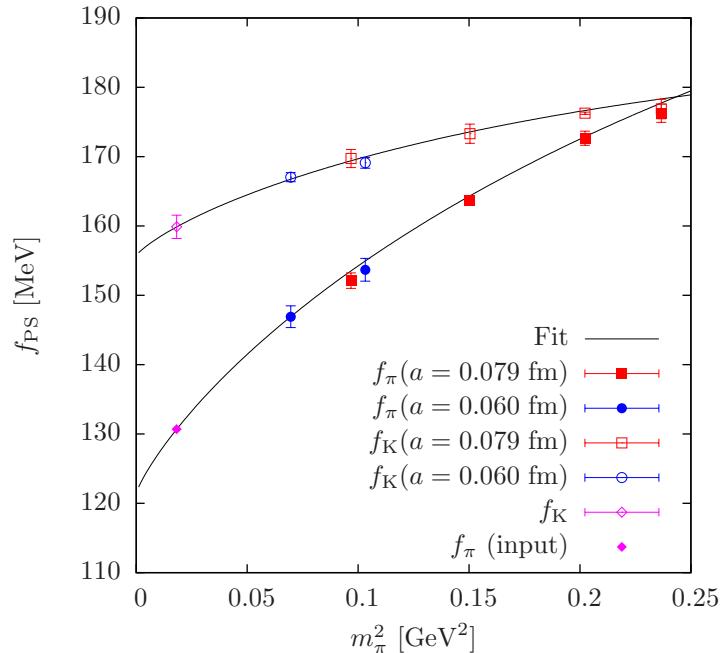
$$f_{\text{PS}}(\mu_\ell, \mu_\ell, \mu_s) = (f_0^{(K)} + f_m^{(K)} \xi_{ss}) \cdot \left[ 1 - \frac{3}{4} \xi_{\ell\ell} \ln \xi_{\ell\ell} + (b_0^{(K)} + b_m^{(K)} \xi_{ss}) \xi_{\ell\ell} \right]$$

$$\xi_{XY} = \frac{m_{\text{PS}}^2(\mu_\ell, \mu_X, \mu_Y)}{(4\pi f_0)^2}$$

(Gasser, Leutwyler (1984); Allton et al (2008); ETMC, Blossier et al. (2010))

- correct for finite size effects using NLO  $\chi$ PT  
(Gasser, Leutwyler (1987); Becirevic, Villadoro (2004))

## $N_f = 2 + 1 + 1$ light quark sector: fit results



- fit  $\beta = 1.95$  ( $a = 0.079\text{fm}$ ) and  $\beta = 2.10$  ( $a = 0.06\text{fm}$ ) simultaneously
- from setting  $m_{PS}^2(\mu_\ell, \mu_s, \mu_s) = 2m_K^2 - m_\pi^2$
- $m_\pi = 135 \text{ MeV}, f_\pi = 130.7 \text{ MeV}, m_K = 497.7 \text{ MeV}$

preliminary fit results:

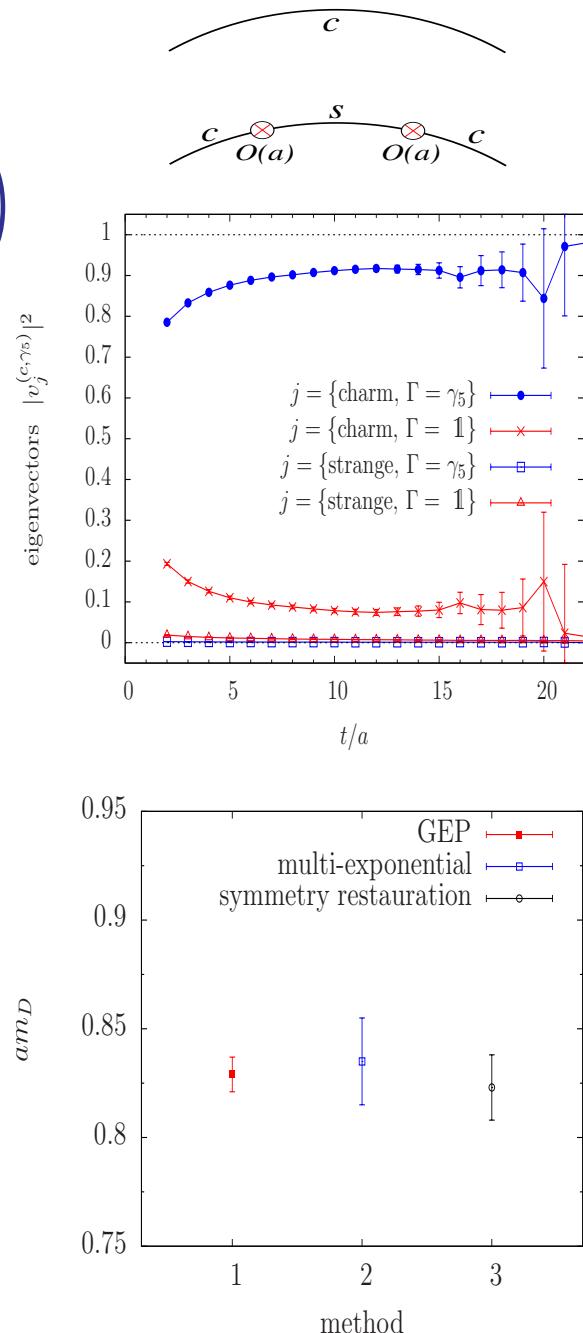
- $f_K/f_\pi = 1.224(13)$ ,  $f_K = 160(2) \text{ MeV}$ ,  $\bar{\ell}_4 = 4.78(2)$ ,  $|V_{us}| = 0.220(2)$
- errors statistical only

$$N_f = 2 + 1 + 1 \text{ heavy quark sector}$$

Wilson twisted mass Dirac operator for  $(c, s)$  pair:

$$D_h = \begin{pmatrix} \gamma_\mu \tilde{\nabla}_\mu + \mu_\sigma + \mu_\delta & i\gamma_5 \left( \frac{a}{2} \nabla_\mu^* \nabla_\mu - m_q \right) \\ i\gamma_5 \left( \frac{a}{2} \nabla_\mu^* \nabla_\mu - m_q \right) & \gamma_\mu \tilde{\nabla}_\mu + \mu_\sigma - \mu_\delta \end{pmatrix}$$

- mixing of  $c$  and  $s$  flavour and of parity
- Kaon is the ground state : good precision
- D meson appears as an excited state
- three independent methods:
  - generalised eigenvalue problem
  - multi-exponential fits
  - imposing parity and flavour restoration at finite  $a$
- they provide consistent results for  $m_D$
- overcome mixing of flavour  $\rightsquigarrow$  mixed action



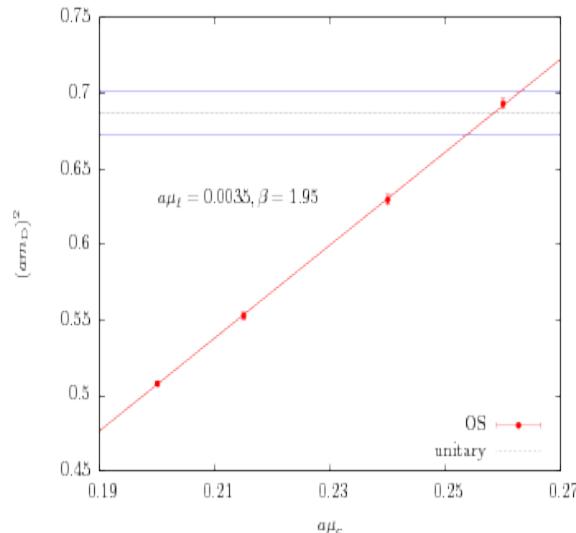
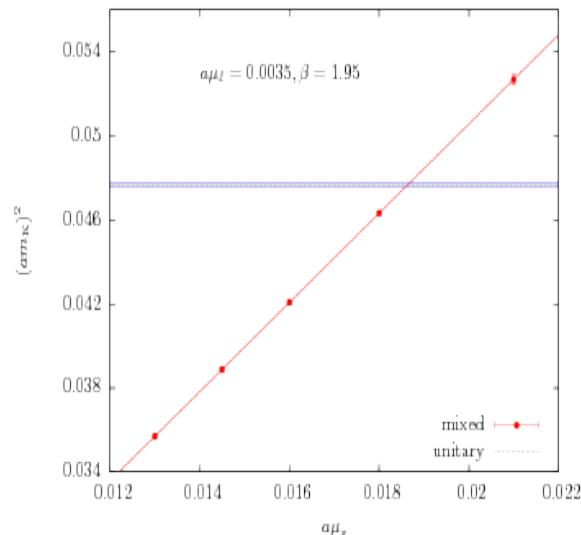
## $N_f = 2 + 1 + 1$ approaching the charm quark

- introduce Wilson twisted mass doublets in the valence sector

$$D_{tm}(\mu_{val}) = D + m_{\text{crit}} + i \mu_{val} \gamma_5 \tau^3$$

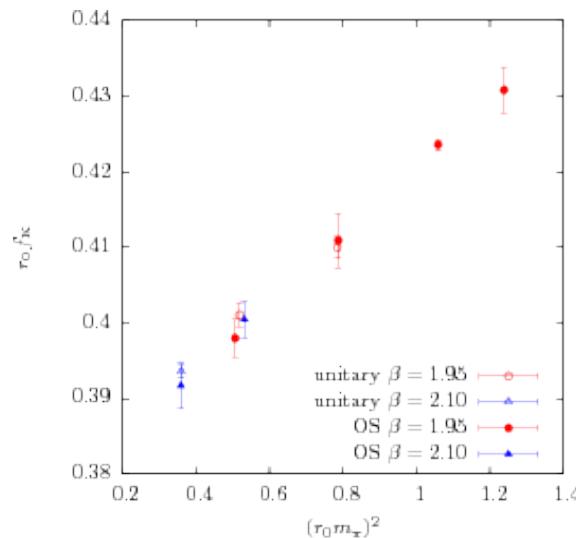
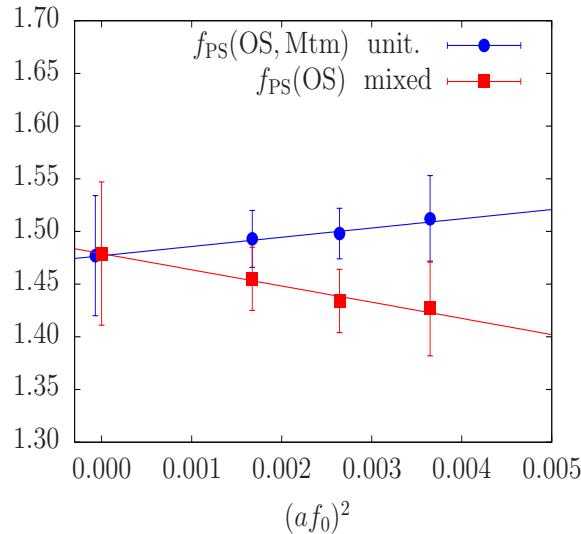
(Osterwalder, Seiler (1990), Pena et al. (2004); Frezzotti, Rossi (2004))

- $m_{\text{crit}}$  from unitary set-up
- 4 – 6 values for  $\mu_{val}$  in the strange  $\mu_s$  and the charm  $\mu_c$  region inversions with multi-mass solver
- matching to unitary set-up using  $m_K$  and  $m_D$
- $\Rightarrow$  avoid flavour breaking



## Unitary versus Osterwalder-Seiler: $f_K$

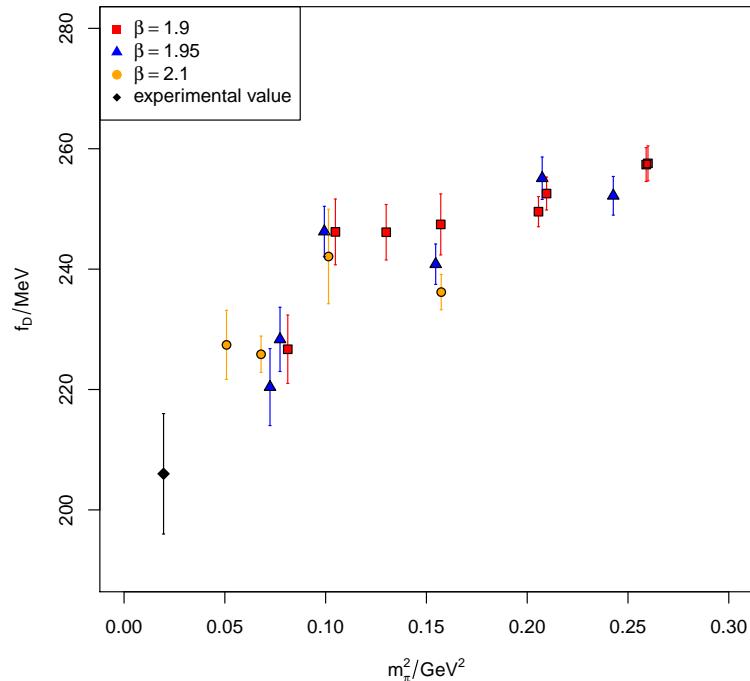
- the unitary  $f_K$  can be computed from:  $f_K = (m_\ell + m_s) \frac{\langle 0 | P_K | K \rangle}{m_K^2}$   
with  $m_s = \mu_\sigma - (Z_P/Z_S)\mu_\delta$
- similar formula for  $f_D$
- $P_K$  is the physical Kaon projecting operator
- the mixed action  $f_K$  computed from:  $f_{\text{PS}} = \left( \mu_{\text{val}}^{(1)} + \mu_{\text{val}}^{(2)} \right) \frac{|\langle 0 | P | PS \rangle|}{m_{\text{PS}} \sinh m_{\text{PS}}}$ ,



Test for  $N_f = 2$

situation for  $N_f = 2 + 1 + 1$

## Decay constants, $F_D$ , $F_{D_s}$



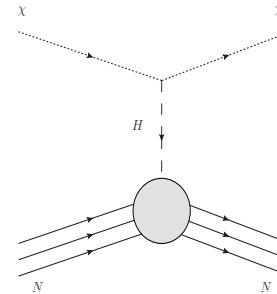
- quark mass dependence of  $f_D$
- input:  $m_\pi = 135 \text{ MeV}$ ,  $f_\pi = 130.7 \text{ MeV}$ ,  $m_K = 497.7 \text{ MeV}$
- all results preliminary

- results very encouraging  
 $f_{D_s} = 250(3) \text{ MeV}$ ,  $f_D = 204(3) \text{ MeV}$ ,  $f_{D_s}/f_D = 1.230(6)$
- very preliminary but very first results from  $N_f = 2 + 1 + 1$  !

# The strange quark content of the nucleon

(Drach, Dinter, Frezzotti, Herdoiza, Rossi, K.J.)

- neutralino in supersymmetric models candidate for dark matter
- interaction with nucleon most strongly through the strange quark content via the Higgs boson exchange diagram



spin independent cross section:

$$\sigma_{\text{SI}} \propto \sum_q \frac{f_{Tq}}{m_q} ; q = u, d, s, c$$

$$f_{Tq} = \frac{\langle N | m_q \bar{q} q | N \rangle}{m_N} \equiv m_q B_q$$

⇒ cross section proportional to quark content; independent from quark mass

Study here:  $\langle N | \bar{s}s | N \rangle = m_N B_s$ ;  $\langle N | \bar{c}c | N \rangle = m_N B_c$

## The problem

spin independent cross section strongly dependend on  
pion-nucleon sigma term  $\Sigma_{\pi N}$

Varying  $48 \text{ MeV} < \Sigma_{\pi N} < 80 \text{ MeV}$

$\Rightarrow$  cross section changes by an order of magnitude

$\Sigma_{\pi N}$  connected to  $y_N$  parameter

$$y_N = \frac{2B_s}{B_u + B_d} ; B_q = \frac{\langle N | \bar{q}q | N \rangle}{m_N}$$

relation:  $y_N = 1 - \sigma_0 / \Sigma_{\pi N}$

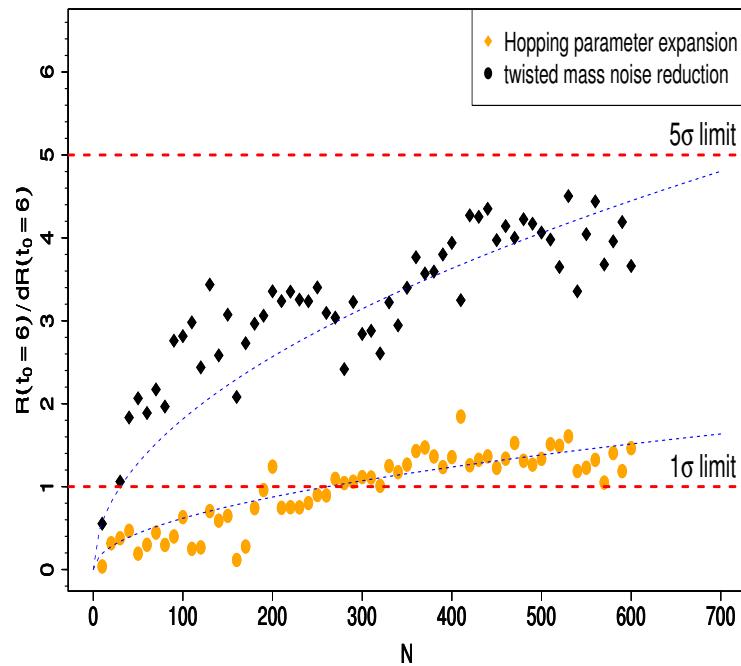
$$\sigma_0 = m_q \langle N | \bar{u}u + \bar{d}d - 2\bar{s}s | N \rangle , \quad m_q = (m_u + m_d)/2$$

from  $\chi$ PT:  $y_N = 0.44(13) \rightarrow$  quite large

want: a first principle, non-perturbative computation of  $f_{T_s}, f_{T_c}$  and  $y_N$

## Twisted mass fermions: special noise reduction technique

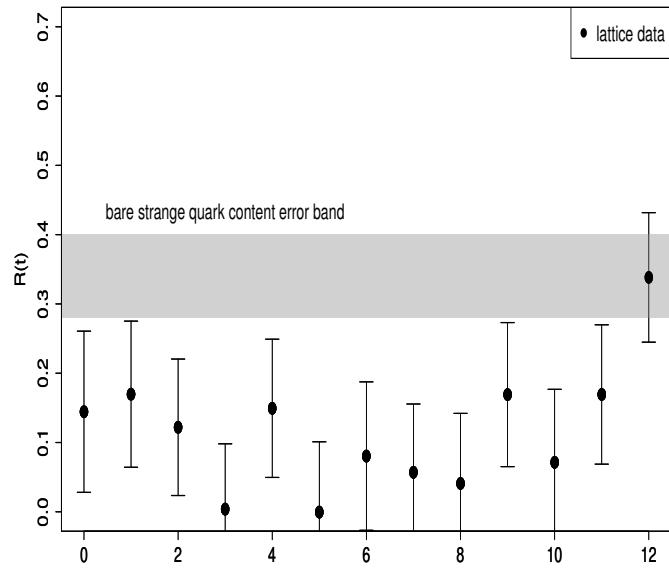
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- standard calculation very (too?) difficult
- using techniques for twisted mass fermions
  - can obtain a signal with reasonable statistics
- remark: calculation of dis-connected contribution to neutral pion mass much easier

## Twisted mass fermions: strange and charm: $\langle N|\bar{s}s|N\rangle$ , $\langle N|\bar{c}c|N\rangle$ ,

- charm quark content



band: plateau value for strange quark content

- $\langle N|\bar{c}c|N\rangle < \langle N|\bar{s}s|N\rangle$  (note: still need multiplication with quark mass)
- $f_{T_s} = 0.011(2)(1)$ ,  $\sigma_0 = 0.137(2)(3)$  MeV,  $y_N = 0.065(12)(2)$   
(note: all results still need extrapolation to physical point)
- still  $y_N^{\text{latt}} \ll y_N^{\text{XPT}}$   $\rightarrow$  bad news for experiments if value persists in chiral limit
- for twisted mass: no mixing effects in renormalization

## Spectral projectors: $\Sigma$ and $\chi_{\text{topo}}$

(Giusti, Lüscher; Lüscher, Palombi; Giusti, Rossi, Testa)

- In the continuum:

$$\frac{\Sigma}{\pi} = \lim_{\lambda \rightarrow 0} \lim_{m \rightarrow 0} \lim_{V \rightarrow \infty} \rho(\lambda, m)$$

$$\rho(\lambda, m) = \frac{1}{V} \sum_{k=1}^{\infty} \langle \delta(\lambda - \lambda_k) \rangle, \quad \Sigma = - \lim_{m \rightarrow 0} \lim_{V \rightarrow \infty} \langle \bar{u}u \rangle$$

- mode number  $\nu \rightsquigarrow$  average number of eigenmodes of  $D_m^\dagger D_m$  with  $\lambda \leq M^2$

$$\nu(M, m) = V \int_{-\Lambda}^{\Lambda} d\lambda \rho(\lambda, m), \quad \Lambda = \sqrt{M^2 - m^2}$$

$$\nu(M, m) = \nu_R(M_R, m_R) \rightsquigarrow \text{renormalization-group invariant}$$

- $\Sigma_R \propto \frac{\partial}{\partial M_R} \nu_R$

## Condensate

- Spectral Projector  $\mathbb{P}_M$  to compute  $\nu(M, m)$

$$\nu(M, m_q) = \langle \text{Tr}\{\mathbb{P}_M\} \rangle$$

- Approximation of  $\mathbb{P}_M$ :

$$\begin{aligned}\mathbb{P}_M &\approx h(\mathbb{X})^4, \\ \mathbb{X} &= \frac{2M^2}{D_m^\dagger D_m + M^2} - 1\end{aligned}$$

- $h(x)$  is an approximation to the step function  $\theta(x)$  in the interval  $[-1, 1]$

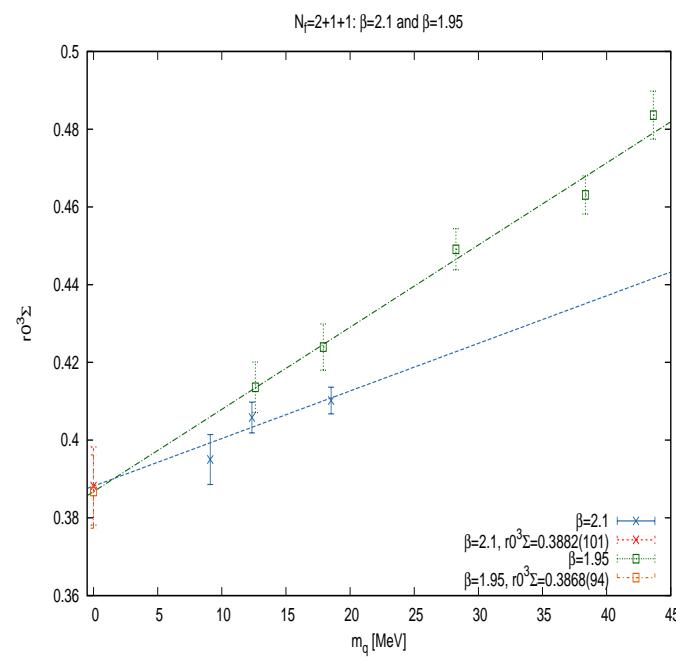
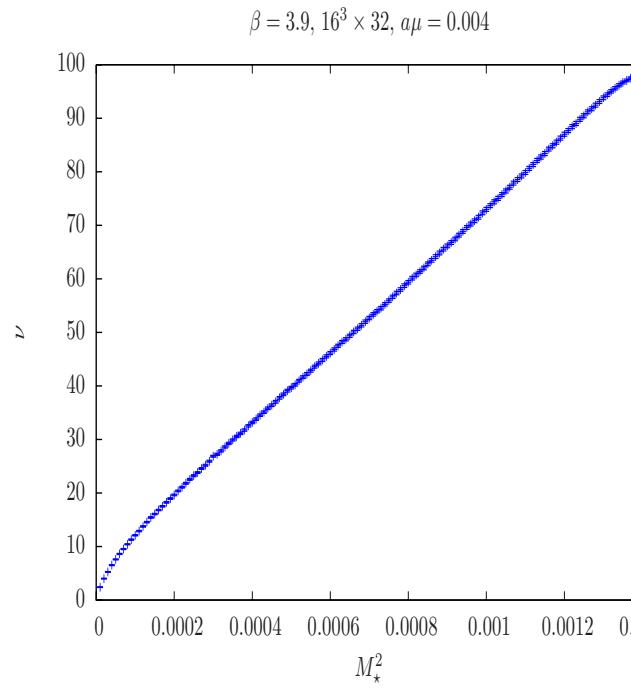
$$h(x) = \frac{1}{2}\{1 - xP(x^2)\}$$

where  $P(x)$  is the polynomial which minimizes  $\delta = \max_{\epsilon \leq y \leq 1} \|1 - \sqrt{y}P(y)\|$

- $\nu(M, m_q) = \langle \mathcal{O}_N \rangle, \quad \mathcal{O}_N = \frac{1}{N} \sum_{k=1}^N (\eta_k, \mathbb{P}_M \eta_k)$   
 $\eta_k$  sources generated randomly

# Chiral limit of scalar condensate

(Cichy, Garcia Ramos, K.J.)



linear behaviour of mode number

slope:  $\Sigma_{\text{spectral}}^{\text{ren}}$

chiral extrapolation of condensate

two lattice spacings

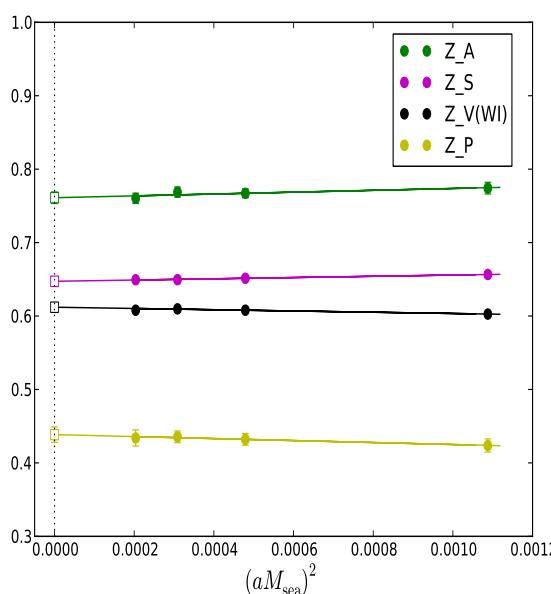
## Non-perturbative renormalization for $N_f = 2 + 1 + 1$

renormalisation factors computed from dedicated  $N_f = 4$  flavour simulations of Wilson fermions

- RI-MOM scheme at non zero values of both the standard and twisted mass parameters

$$M_R = \frac{1}{Z_P} \sqrt{(Z_A m_{\text{PCAC}})^2 + \mu_q^2} \rightarrow 0$$

- $O(a)$  improvement via average of simulations with  $+m_{\text{PCAC}}$  and  $-m_{\text{PCAC}}$



study at  $\beta = 1.95$

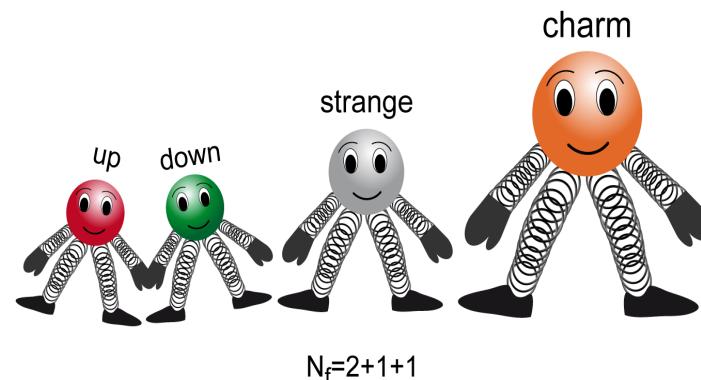
$a = 0.08 \text{ fm}, L = 1.9 \text{ fm}$

- linear mass dependence
- allows for chiral extrapolation

## Simulation setup for $N_f = 2 + 1 + 1$ Configurations available through **ILDG**

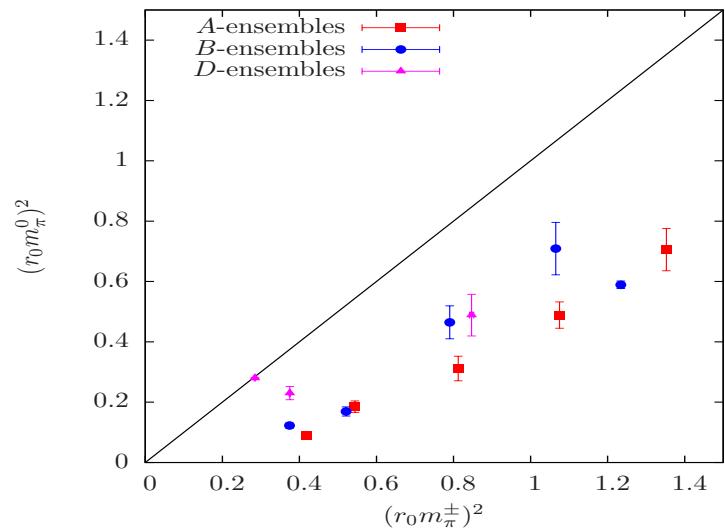
$\beta$	$a[\text{fm}]$	$L^3 T/a^4$	$m_\pi [\text{MeV}]$	therm/production
1.9	$\approx 0.085$	$24^3 48$	300 – 500	1500/5000
1.95	$\approx 0.075$	$32^3 64$	300 – 500	1500/5000
2.0	$\approx 0.065$	$32^3 64$	300	1500/5000
2.1	$\approx 0.055$	$48^3 96$	230 – 500	1500/5000

- can go down to  $m_\pi \approx 230\text{MeV}$
- see only small lattice spacing scaling
- can perform rich physics programme



## Size of cut-off effects: pion mass splitting

- question: how fast can we reach the physical point?



- Preliminary!
  - $m_\pi^0 < m_\pi^\pm \rightarrow c_2 < 0$
- significant flavour violations

- answer: not fast enough!

## Effects of smearing for $N_f = 2 + 1 + 1$

action	$a\mu_\ell$	$\kappa_{\text{crit}}$	$Z_V[\text{WI}]$	$Z_P/Z_S$
0-stout	0.0060	0.163265	0.60	0.67
	0.0080	0.163260		
	0.0080	0.163204		
1-stout	0.0060	0.145511	0.73	0.77
	0.0080	0.145510		
4-stout	0.0015	0.136720	0.82	0.86

- $\kappa_{\text{crit}} \rightarrow$  moves closer to  $1/8$
- $Z$  factors  $\rightarrow$  move closer to 1
- plaquette behaves much smoother:

$$\left. \frac{\Delta[\langle P \rangle]}{\Delta[(2\kappa)^{-1}]} \right|_{\kappa_{\text{crit}}} = 11.4(\text{no stout}) \rightarrow -3.4(\text{stout})$$

- proof-tested that simulations at  $m_\pi/f_\pi = \text{physical}$  feasible at lattice spacing  $a \approx 0.1\text{fm}$

## Summary

- **ETMC** successful simulations with  $N_f = 2$  and  $N_f = 2 + 1 + 1$  quark flavour
  - found good scaling behaviour
  - could achieve accurate results for many quantities
  - performed dedicated renormalization programme
- simulation at physical point difficult with present action
- developed new (maximally) twisted mass action
  - reach  $m_\pi/f_\pi = \text{physical}$  at lattice spacing  $a \approx 0.1\text{fm}$
  - $m_\pi^0 \approx m_\pi^\pm$
- plan new simulations at physical point (+isospin + electromagnetism)